MOBILITY OF POSITIVE IONS IN THEIR OWN GAS:

DETERMINATION OF AVERAGE MOMENTUM-TRANSFER CROSS SECTION

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Lewis Research Center
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SUMMARY

The energy-dependent charge exchange cross section is integrated over the appropriate energy distribution to yield the average momentum cross section for an ion in its own gas. This momentum cross section $\overline{Q}$ is presented in terms of charge exchange constants A and B, numerical constants $\mathcal{E} = 0.577...$ and $\mathcal{K} = 2.492...$, the atomic polarizability α, and the thermal energy of the gas kT. The expression

$$\overline{Q} = 2A^2 - 4AB\left(\frac{3}{2} - \mathcal{E} + \ln kT\right) + B^2\left[4\left(\frac{3}{2} - \mathcal{E}\right)\ln kT + 2(\ln kT)^2 + \mathcal{K}\right]$$

$$+ \frac{\pi}{2}\frac{e^2\alpha}{B^2 kT\left(\frac{A}{B} - \ln kT\right)^2}$$

is obtained herein and is shown to have an error $\Delta\overline{Q}/\overline{Q}$ of less than $1.15\ \alpha/[(AB)^2 + 5\alpha]$.

The average momentum cross section obtained from this equation can be used to compare energy-dependent charge exchange cross section data with mobility data; this is illustrated by an example for several inert gas ions in their own gas. The average momentum cross section has also been used to compute the mobility of alkali-metal ions in their own vapor. The calculations reveal errors in earlier numerical approaches.

INTRODUCTION

When the mobilities of positive ions in their own gases are calculated, three problems must be solved:

(1) Ion motion must be analyzed by using kinetic theory.

(2) The energy-dependent momentum-transfer cross section for the ion in its own gas must be computed.

(3) The energy-dependent momentum-transfer cross section obtained in problem (2) must be integrated over an appropriate energy distribution dictated by problem (1).

The solution of problem (1) is presented in classical texts on kinetic theory (refs. 1 and 2) for the case of low applied electric fields, a condition to which the present analysis is restricted.

Many authors (e.g., refs. 3 to 6) agree on the general solution to problem (2) for low collision energies (below 100 ev). This 100-electron-volt energy limitation is compatible with the low-field restriction on problem (1).

This report is primarily concerned with the solution to problem (3). While previous numerical (ref. 7) or empirical (ref. 8) approaches are adequate for specific instances, they do not permit observance of the dependence of ion mobility on the various parameters significant to the mobility problem (atomic polarizability, gas temperature, and charge exchange constants). Furthermore, they entail considerable time and labor with each application. The required integration is carried out herein through the use of appropriate approximations. The resulting dependence of the ion mobility on the various parameters appearing in the problem thus becomes clear.

MOBILITY AND MOMENTUM-TRANSFER CROSS SECTION

The theory of ion mobility in the low-field limit (ref. 9) is concerned with the motion of thermalized ions across a region of uniform electric field E. The motion is inhibited by a gas of considerably greater particle density N than the ion density. (Ion-ion interactions can be neglected.) The low-field limit implies that the velocity of the ions acquired by acceleration in the field between collisions is less than their thermal velocity. The average velocity of the ions in the direction of the applied electric field is defined as the drift velocity v_D.

Measurements of ion drift velocity are usually reported in terms of ion mobility μ, defined by

$$\mu \equiv \frac{v_D}{E}$$

plotted against the ratio E/P, where P is gas pressure for constant gas temperature T. (Symbols are defined in appendix A.) The physical significance of E/P becomes apparent by use of the gas law

$$P = NkT$$

and the definition of mean free path λ

$$\lambda = \frac{1}{N\bar{\sigma}}$$

where $\bar{\sigma}$ is the ion-atom collision cross section averaged over an appropriate energy distribution. Therefore

$$\frac{E}{P} = \frac{E\bar{\sigma}}{\bar{\sigma}NkT} = \frac{eE\lambda}{kT} \frac{\bar{\sigma}}{e}$$

where e is the electron charge, and kT is the average thermal energy of the ion. The quantity $eE\lambda$ is the average energy gained by the ion from the electric field between collisions. Hence, E/P is proportional to the ratio of directed energy derived from the applied electric field to the random energy of thermal motion.

Townsend (ref. 10) has shown that the relation between ion mobility μ in an electric field and ion motion due to diffusion across a concentration gradient is given by

$$\mu = \frac{eD}{kT} \tag{1}$$

where D is the diffusion coefficient.

Chapman (refs. 11 and 12) and Enskog (ref. 13) obtained an expression for this diffusion coefficient. (Their work is presented in more recent texts by Chapman and Cowling (ref. 1) and Hirschfelder et al. (ref. 2).) The Chapman-Enskog procedure is to obtain an approximate solution to the Boltzmann equation for nonequilibrium conditions by a perturbation technique. The Chapman-Enskog results inserted into equation (1) with the restriction that the ions and gas atoms are the same element yield

$$\mu = \frac{3\sqrt{\pi}}{8} \frac{e}{\sqrt{mkT} \ N\bar{Q}} \tag{2}$$

where m is the ion or atom mass and

$$\bar{Q} = \frac{1}{2(kT)^3} \int_0^\infty \epsilon^2 Q(\epsilon) e^{-\epsilon/kT} \, d\epsilon \tag{3}$$

Here ϵ is the relative kinetic energy of an ion with respect to a gas atom and $Q(\epsilon)$ is the energy-dependent momentum-transfer cross section for an ion-atom collision.

The relation between momentum-transfer cross section and resonant charge exchange cross section $\sigma_X(\epsilon)$ is (refs. 14 and 15)
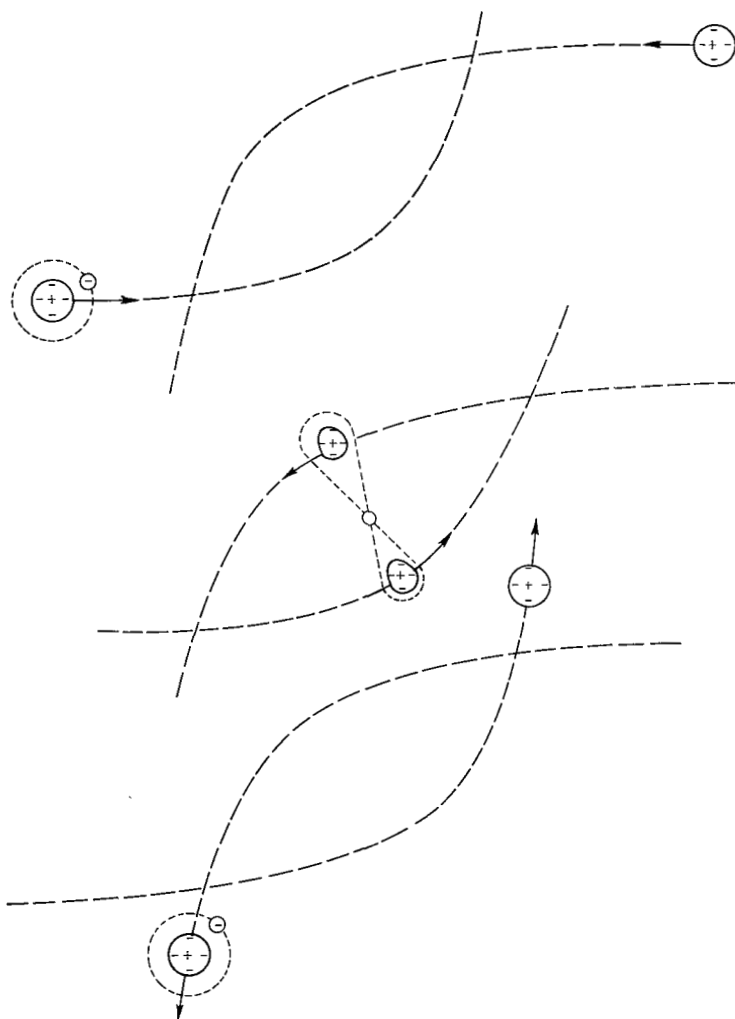
$$Q(\epsilon) = 2\sigma_X(\epsilon) \tag{4}$$

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Resonance charge exchange is the process by which an ion passing an atom of the same element gains one of its outer atomic electrons (fig. 1). This interaction appears to be an elastic scattering at approximately $180°$ in the center-of-mass frame of reference and therefore is a major consideration in charge transport calculations.

The energy dependence of $\sigma_x(\epsilon)$ has been discussed by many authors (e.g., refs. 3 to 6), any of whose results can be approximated by (ref. 7)

$$\sigma_x(\epsilon) = (A - B \ln \epsilon)^2$$

$$\times \left[1 + e^2 \alpha \left(\frac{\pi}{2}\right)^2 \frac{1}{\epsilon(A - B \ln \epsilon)^4} \right]$$

$$(5)$$

where A and B are constants dependent on atomic structure and α is the atomic polarizability. For most gases and vapors, A is between 5 and 50 $\mathring{A}$ and B is between 0.1 and 5 $\mathring{A}$ per $\ln(ev)$ and the ratio A/B is usually greater than 10.0; α ranges from 0.1 to 75 $\mathring{A}^3$. Equation (5) is restricted to energies below some maximum ϵ_m of the order of 100 electron volts (ref. 3). Since ion-atom energies this high or higher are unlikely under thermal conditions and since $\sigma_x(\epsilon)$ is very small above 100 electron volts, the upper limit of integration in equation (3) may be replaced by ϵ_m.

Figure 1. - Ion-neutral elastic scattering event with charge exchange.

AVERAGING THE MOMENTUM-TRANSFER CROSS SECTION

It can be seen from the previous section that the mobility problem can be reduced to one of determining the average momentum cross section by integration of

$$\overline{Q} = \frac{1}{2(kT)^3} \int_0^{\epsilon_m} \epsilon^2 Q(\epsilon) e^{-\epsilon/kT} \, d\epsilon \qquad (6)$$

where $Q(\epsilon)$ is given by the combination of equations (4) and (5):

$$Q(\epsilon) = 2(A - B \ln \epsilon)^2 \left[1 + e^2 \alpha \left(\frac{\pi}{2} \right)^2 \frac{1}{\epsilon(A - B \ln \epsilon)^4} \right] \qquad (7)$$

Equation (7) may be inserted into equation (6) and the result written

$$\overline{Q} = \left(\frac{1}{kT} \right)^3 \left[I_1 + \left(\frac{\pi}{2} \right)^2 \frac{e^2 \alpha}{B^2} I_2 \right] \qquad (8)$$

where

$$I_1 \equiv \int_0^{\epsilon_m} e^{-\epsilon/kT} \epsilon^2 \times (A - B \ln \epsilon)^2 \, d\epsilon \qquad (9)$$

and

$$I_2 \equiv \int_0^{\epsilon_m} e^{-\epsilon/kT} \frac{\epsilon}{\left(\frac{A}{B} - \ln \epsilon \right)^2} \, d\epsilon \qquad (10)$$

Figure 2. – Integrand of I_1. $I_1 = \int_0^{\epsilon_m} g_1(\epsilon) d\epsilon$.

Determination of I_1

The behavior of the integrand of I_1, $g_1(\epsilon)$, above ϵ_m has no physical significance (fig. 2); but, because it is always quite small, the upper limit of integration of equation (9) can be extended to infinity without introducing serious error.

With the definitions $a \equiv e^{A/B}$ and $x \equiv \epsilon/kT$, equation (9) becomes

$$I_1 = B^2 (kT)^3 \left[\left(\ln \frac{kT}{a} \right)^2 \int_0^\infty x^2 e^{-x} \, dx + 2 \ln \frac{kT}{a} \int_0^\infty x^2 (\ln x) e^{-x} \, dx \right.$$

$$\left. + \int_0^\infty x^2 (\ln x)^2 e^{-x} \, dx \right] \qquad (11)$$

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The three definite integrals were determined with the aid of Bierens de Haan's Integral Tables (ref. 16). The first is

$$\int_0^\infty x^2 e^{-x}\, dx = 2 \tag{12}$$

The second is

$$\int_0^\infty x^2 (\ln x) e^{-x}\, dx = \Gamma(3) \psi^B(3) \tag{13}$$

where $\Gamma(q)$ is the gamma function and $\psi^B(q)$ is Bateman's psi function (ref. 17). For the specific case of $q = 3$, $\psi^B(3) = \frac{3}{2} - \mathcal{E}$, where $\mathcal{E}$ is Euler's constant, $0.5772\ldots$ (see appendix B). The third integral is

$$\int_0^\infty x^2 (\ln x)^2 e^{-x}\, dx = \left[\frac{d^2 \Gamma(q)}{dq^2} \right]_{q=3} \tag{14}$$

where

$$\left[\frac{d^2 \Gamma(q)}{dq^2} \right]_{q=3} = \mathcal{K} = 2.492\ldots$$

(see appendix B).

Combining equations (11) to (14) yields

$$I_1 = B^2 (kT)^3 \left[2\left(\ln \frac{kT}{a} \right)^2 + 4\left(\ln \frac{kT}{a} \right)\left(\frac{3}{2} - \mathcal{E} \right) + \mathcal{K} \right] \tag{15}$$

Determination of I_2

Equation (10) can be written as

$$I_2 = \int_0^{\epsilon_m} \epsilon^{-\epsilon/kT} \frac{\epsilon\, d\epsilon}{\left(\ln \frac{\epsilon}{a} \right)^2}$$

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The integrand of I_2, $g_2(\epsilon)$, is shown in figure 3. Note the sharp dis-
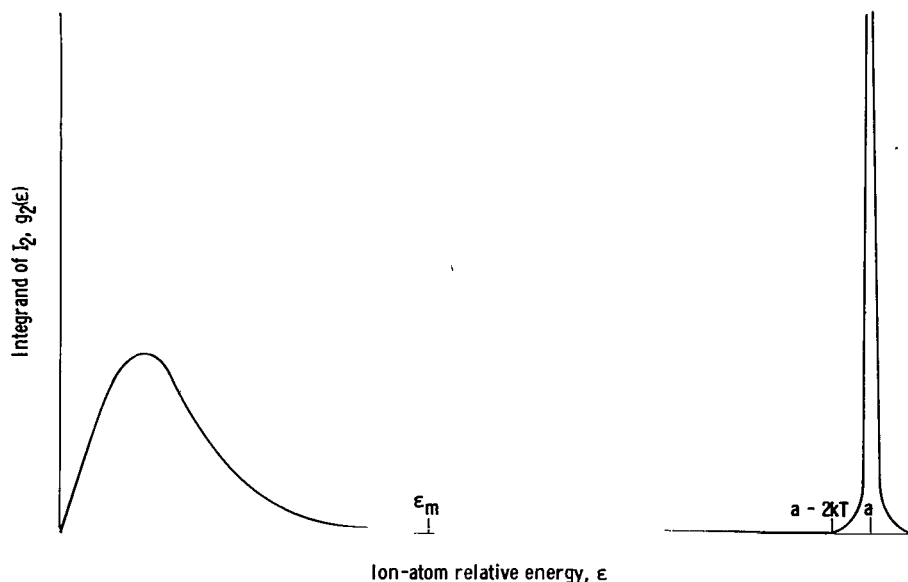

Figure 3. - Integrand of I_2. $I_2 = \int_0^{\epsilon_m} g_2(\epsilon)d\epsilon$.

continuity at $\epsilon = a$. The discontinuity is sharpened by the occurrence of a minimum at $\epsilon \simeq a - 2kT$. Typical values of a are above 10,000 electron volts, while kT is between 0.01 and 0.25 electron volt (115° K$< T < 3000^{\circ}$ K). The discontinuity has no physical significance, since the cross-section expression being integrated does not represent the physical phenomena above $\epsilon_m \simeq 100$ electron volts (ref. 3).

A convenient procedure for obtaining an approximate value for I_2 is to apply the quadrature formula (ref. 18)

$$\int_0^\infty x^\beta e^{-x} f(x)\ dx \simeq \sum_{i=1}^n \mathscr{A}_i f(x_i) \qquad (16)$$

where the nodes are the roots of the Chebyshev-Laguerre polynomial $L_n^{(\beta)}(x)$, that is,

$$L_n^{(\beta)}(x) = (-1)^n x^{-\beta} e^x \frac{d^n}{dx^n} x^{\beta+n} e^{-x}$$

where

$$L_n^{(\beta)}(x_i) = 0$$

is required.

The coefficient $\mathscr{A}_i$ is

$$\mathscr{A}_i = \frac{n!\,\Gamma(\beta + n + 1)}{x_i\left[\dfrac{dL_n^{(\beta)}(x)}{dx}\bigg|_{x=x_i}\right]^2}$$

If the continuous function

$$f(x) = \frac{x}{\left(\dfrac{A}{B} - \ln xkT\right)^2}$$

is used for $0 \leq x \leq x_m$, and $f(x)$ goes smoothly and quickly to zero for $x_m < x \leq \infty$, then

$$I_2 = (kT)^2\left[\int_0^\infty e^{-x}f(x)dx - \int_{x_m}^\infty e^{-x}f(x)dx\right]$$

where $x = \epsilon/kT$. Since $x_m > 300$,

$$I_2 \simeq (kT)^2 \int_0^\infty e^{-x}f(x)dx$$

When equation (16) is applied for $\beta = 0$ and the inaccuracy of a single-node approximation ($n = 1$) is accepted,

$$I_2 \simeq \frac{(kT)^2}{\left(\dfrac{A}{B} - \ln kT\right)^2} \tag{17}$$

Since the term in equation (8) that includes I_2 is generally less than 25 percent of $\overline{Q}$ for temperatures above 50° K, equation (17) should be a sufficiently good approximation for most applications. The average momentum cross section can now be expressed

$$\overline{Q} \simeq 2A^2 - 4AB\left(\frac{3}{2} - \mathscr{E} + \ln kT\right) + B^2\left[4\left(\frac{3}{2} - \mathscr{E}\right)\ln kT + 2(\ln kT)^2 + \mathscr{K}\right]$$

$$+ \left(\frac{\pi}{2}\right)^2 \frac{e^2\alpha}{B^2 kT\left(\dfrac{A}{B} - \ln kT\right)^2} \tag{18}$$

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DISCUSSION

Error in Determination of I_1

The extension of the upper limit of integration of I_1 from ϵ_m to infinity introduces an error ΔI_1 into the determination of I_1. The magnitude of the fractional error $\Delta I_1/I_1$ may be expressed by

$$\frac{\Delta I_1}{I_1} = \cfrac{1}{\cfrac{\displaystyle\int_0^\infty g_1(\epsilon)d\epsilon}{\displaystyle\int_{\epsilon_m}^\infty g_1(\epsilon)d\epsilon} - 1}$$

Noting that

$$\int_{\epsilon_m}^\infty g_1(\epsilon)d\epsilon < B^2 \left(\ln \frac{\epsilon_m}{a}\right)^2 \int_{\epsilon_m}^\infty \epsilon^2 e^{-\frac{\epsilon}{kT}} d\epsilon$$

and using equation (15) produce

$$\frac{\displaystyle\int_0^\infty g_1(\epsilon)d\epsilon}{\displaystyle\int_{\epsilon_m}^\infty g_1(\epsilon)d\epsilon} > \cfrac{\left[2\left(\ln\frac{kT}{a}\right)^2 + 4\left(\ln\frac{kT}{a}\right)(3/2 - \mathcal{E}) + \mathcal{K}\right]}{e^{-\frac{\epsilon_m}{kT}}\left(\ln\frac{\epsilon_m}{a}\right)^2\left[\left(\frac{\epsilon_m}{kT} + 1\right)^2 + 1\right]}$$

Further approximations that strengthen the inequality yield

$$\frac{\displaystyle\int_0^\infty g_1(\epsilon)d\epsilon}{\displaystyle\int_{\epsilon_m}^\infty g_1(\epsilon)d\epsilon} > \cfrac{2e^{\frac{\epsilon_m}{kT}}}{\left[\left(\frac{\epsilon_m}{kT} + 1\right)^2 + 1\right]}$$

Now the maximum error in I_1 is limited by

$$\frac{\Delta I_1}{I_1} < \left[\left(\frac{\epsilon_m}{kT} + 1\right)^2 + 1\right]e^{-\frac{\epsilon_m}{kT}}$$

When $kT \simeq 0.3$ electron volt and $\epsilon_m = 100$ electron volts, $\Delta I_1/I_1 < 10^{-140}$.

Error in Determination of I_2

The largest error in this calculation is the result of using the single-node quadrature formula. A two-node quadrature gives (ref. 18)

$$I_2 = (kT)^2 \left\{ \frac{0.5000}{\left[\frac{A}{B} - \ln(0.5858\ kT)\right]^2} + \frac{0.4998}{\left[\frac{A}{B} - \ln(3.414\ kT)\right]^2} \right\} \tag{19}$$

and a three-node quadrature gives

$$I_2 = (kT)^2 \left\{ \frac{0.2957}{\left[\frac{A}{B} - \ln(0.4158\ kT)\right]^2} + \frac{0.6390}{\left[\frac{A}{B} - \ln(2.294\ kT)\right]^2} + \frac{0.0654}{\left[\frac{A}{B} - \ln(6.290\ kT)\right]^2} \right\} \tag{20}$$

As the number of nodes used in the calculation is increased, the exact value can be approached with a greater degree of accuracy. A comparison of one-, two-, and three-node approximations (eqs. (17), (19), and (20)) is given in the following table:

kT, ev	$\frac{A}{B}$, $\ln$(ev)	Approximation of I_2		
		One node	Two node	Three node
0.001	20	1.380×10^{-9}	1.422×10^{-9}	1.425×10^{-9}
.100	20	2.011×10^{-5}	2.083×10^{-5}	2.091×10^{-5}
.001	5	7.031×10^{-9}	7.538×10^{-9}	7.591×10^{-9}
.100	5	1.877×10^{-4}	2.167×10^{-4}	2.185×10^{-4}

An estimate of the maximum error ΔI_2 introduced by the single-node approximation can be obtained from the determination of an upper and a lower limiting value of I_2, $(I_2)_{max}$ and $(I_2)_{min}$.

Since $[1/\ln\,(\epsilon/a)]^2$ increases monatonically from zero at $\epsilon = 0$ to $[1/\ln\,(\epsilon_m/a)]^2$ at ϵ_m, I_2 can be no greater than

$$(I_2)_{max} = \sum_{n=0}^{N} \left(\frac{1}{\ln \frac{\epsilon_{n+1}}{a}}\right)^2 \int_{\epsilon_n}^{\epsilon_{n+1}} \epsilon e^{-\epsilon/kT}\, d\epsilon + \frac{\epsilon_{N+1}\, e^{-\frac{\epsilon_{N+1}}{kT}}\ \epsilon_m}{\left(\ln \frac{\epsilon_{N+1}}{a}\right)^2}$$

and no less than

$$(I_2)_{min} = \sum_{n=0}^{N} \left(\frac{1}{\ln \frac{\epsilon_n}{a}}\right)^2 \int_{\epsilon_n}^{\epsilon_{n+1}} \epsilon e^{-\frac{\epsilon}{kT}} d\epsilon$$

If equal energy intervals of kT are chosen,

$$(I_2)_{max} = \left(\frac{kT}{\ln \frac{kT}{a}}\right)^2 \left\{ \sum_{n=0}^{N} \left[\frac{\ln \frac{kT}{a}}{\ln \frac{(n+1)kT}{a}}\right]^2 (n+1)\left(1 - \frac{1}{e}\frac{n+2}{n+1}\right) e^{-n} \right.$$

$$\left. + (N+1)e^{-(N+1)} \left[\frac{\ln \frac{kT}{a}}{\ln \frac{(N+1)kT}{a}}\right]^2 \frac{\epsilon_m}{kT} \right\}$$

and

$$(I_2)_{min} = \left(\frac{kT}{\ln \frac{kT}{a}}\right)^2 \sum_{n=0}^{N} \left(\frac{\ln \frac{kT}{a}}{\ln \frac{nkT}{a}}\right)^2 (n+1)\left(1 - \frac{1}{e}\frac{n+2}{n+1}\right) e^{-n}$$

When $N = 20$ is used along with $kT \geq 0.01$ electron volt,

$$(I_2)_{max} = 1.185 \left(\frac{kT}{\ln \frac{kT}{a}}\right)^2$$

and

$$(I_2)_{min} = 0.772 \left(\frac{kT}{\ln \frac{kT}{a}}\right)^2$$

Hence

$$\left|\frac{\Delta I_2}{I_2}\right| < 0.23$$

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From equations (2), (8), and (18) the following error in average momentum cross section $\Delta\bar{Q}/\bar{Q}$ and mobility $\Delta\mu/\mu$ is obtained:

$$\left|\frac{\Delta\bar{Q}}{\bar{Q}}\right| = \left|\frac{\Delta\mu}{\mu}\right| < \frac{1.15\,\alpha}{(AB)^2 + 5\alpha}$$

Comparison with Previous Calculations

The mobility expression, equation (2), and the approximate average momentum cross section, equation (18), were used to calculate the mobility of alkali-metal ions in their own vapor at 300° K. The standard vapor density, 2.69×10^{19} atoms per cubic centimeter, was used. The results of these calculations are compared with values obtained by numerical integration (ref. 7) in the following table:

Element	Atomic polarizability, α, $\overset{\circ}{A}^3$	Constant, A, $\overset{\circ}{A}$	Constant, B, $\overset{\circ}{A}/\ln(ev)$	Ion mobility, μ, sq cm/(v)(sec)	
				Eqs. (2) and (18)	Ref. 7
Cesium	61	23.97	1.50	0.0784±0.0034	0.0736
		22.52	1.15	.0914±0.0066	.0880
		31.62	3.12	.0401±0.0003	.0361
		27.40	1.84	.0603±0.0015	.0552
Potassium	36	23.02	1.53	0.157±0.005	0.144
		31.32	3.02	.0765±0.0034	.0683
Rubidium	40	13.22	0.601	0.243±0.042	0.324
Sodium	20	11.40	0.496	0.652±0.114	0.848

The maximum error $\Delta\mu$ in the calculated mobility is also presented. When the two values of μ in the previous table differ by more than $\Delta\mu$, the discrepancy must be attributed to inaccuracy of previously reported numerical results.

Element	Constant, A, $\overset{\circ}{A}$	Constant, B, $\overset{\circ}{A}/\ln(ev)$	Atomic polarizability, α, $\overset{\circ}{A}$ (a)
Helium	[b]5.27	[b]0.320	0.206
Neon	[c]5.76	[c].397	.398
Argon	[d]7.15	[d].441	1.63

[a]Ref. 19.
[b]Ref. 20.
[c]Ref. 21.
[d]Ref. 22.

Comparison of Cross Section and Mobility Experiments

Calculation of temperature-dependent mobility from charge exchange constants A and B provides a basis for comparing charge exchange cross section measurements with mobility measurements. As an example, this comparison is now presented for three inert gas ions in their own vapor. The

cross section data (refs. 21 and 22) have been fitted to a curve of the form of equation (5); the resulting values of A and B are presented in the previous table along with values of α obtained from reference 22.

The constants A and B were inserted in equation (2) and (18) and the resulting temperature-dependent mobilities of helium, neon, and argon ions in their own gas are presented in figure 4. The mobility measurements of refer-
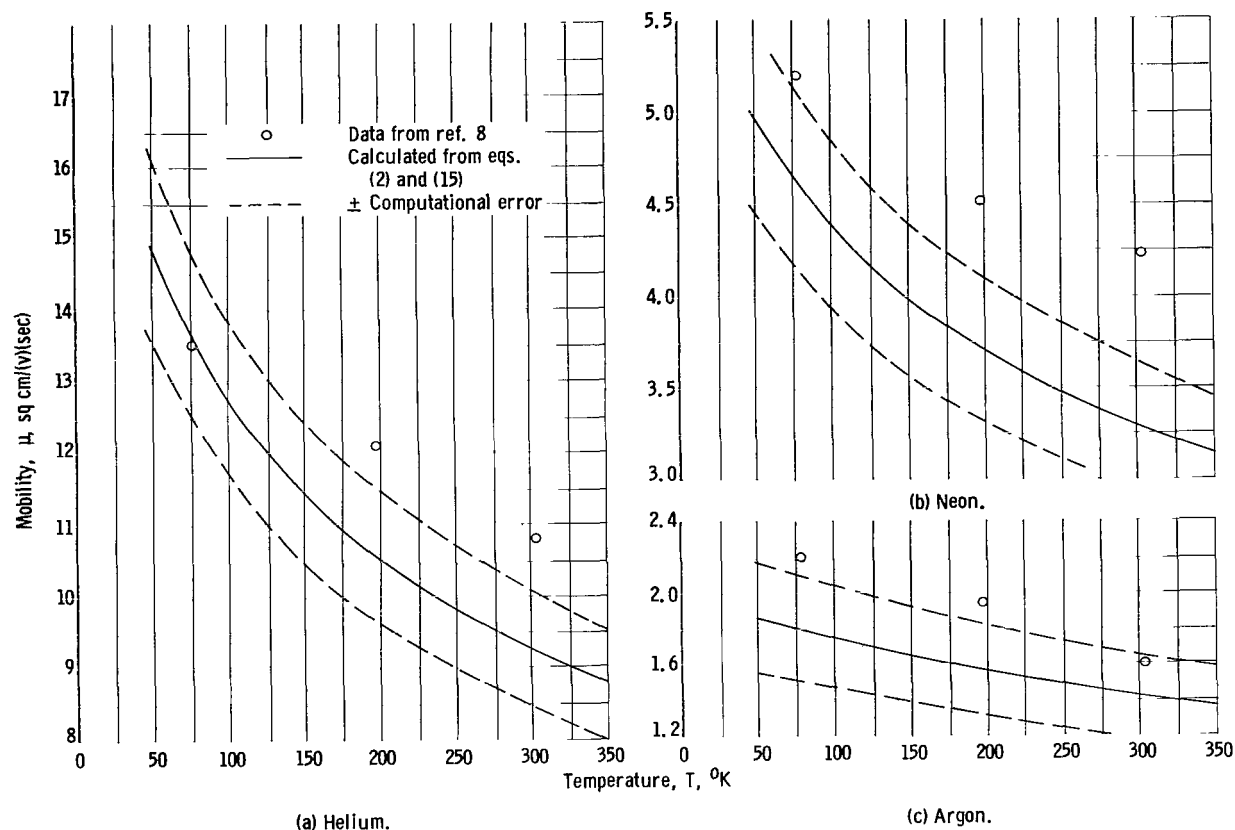

Figure 4. - Mobilities of ions in their own gases.

ence 8 are also presented in this figure for comparison. Measured mobilities outside the band of maximum computational error must be interpreted as a disagreement between the mobility data and the experimental charge exchange cross section data.

CONCLUDING REMARKS

The momentum cross section $\overline{Q}$ can be presented in terms of charge exchange constants A and B, numerical constants $\mathcal{E} = 0.577...$ and $\mathcal{K} = 2.492...$, the atomic polarizability α, and the thermal energy of the gas kT. The expression

$$\overline{Q} = 2A^2 - 4AB\left(\frac{3}{2} - \mathcal{E} + \ln kT\right) + B^2\left[4\left(\frac{3}{2} - \mathcal{E}\right)\ln kT + 2(\ln kT)^2 + \mathcal{K}\right]$$

$$+ \left(\frac{\pi}{2}\right)^2 \frac{e^2 \alpha}{B^2 kT\left(\dfrac{A}{B} - \ln kT\right)^2}$$

has been obtained herein and shown to have an error $\Delta\overline{Q}/\overline{Q}$ of less than $1.15\,\alpha/[(AB)^2 + 5\alpha]$. This equation is subject to the limitations $A/B > 10$ and 0.01 ev $< kT < 0.3$ ev.

The use of this equation and cross section data to obtain the mobility of alkali-metal ions in their own vapor revealed errors in earlier numerical calculations.

The average momentum cross section given by equation (15) can conveniently be used to compare energy-dependent charge exchange cross section data with mobility data; this was illustrated by an example for several inert gas ions in their own gas.

Lewis Research Center
    National Aeronautics and Space Administration
        Cleveland, Ohio, May 11, 1964

SYMBOLS

A,B   constants in expression for theoretical energy-dependent charge exchange
       cross section

$\mathscr{A}_i$ coefficient in quadrature formula

a $e^{A/B}$

D   diffusion coefficient

E   electric field

$\mathscr{E}$ Euler's constant, $0.5772\ldots$

e   electron charge

f   functional dependence in quadrature formula

g_1 integrand of I_1, $e^{-\frac{\epsilon}{kT}}\epsilon^2(A - B \ln \epsilon)^2$

g_2 integrand of I_2, $e^{-\frac{\epsilon}{kT}} \dfrac{\epsilon}{\left(\dfrac{A}{B} - \ln \epsilon\right)^2}$

I_1 value of integral $\displaystyle\int_0^{\epsilon_m} e^{-\frac{\epsilon}{kT}}\epsilon^2(A - B \ln \epsilon)^2 \, d\epsilon$

I_2 value of integral $\displaystyle\int_0^{\epsilon_m} e^{-\frac{\epsilon}{kT}} \dfrac{\epsilon \, d\epsilon}{\left(\dfrac{A}{B} - \ln \epsilon\right)^2}$

k   Boltzmann's constant

L_n Chebyshev-Lagnerre polynomial

m   ion or atom mass

N   gas density

n   summation index in obtaining limiting values of I_2

P	gas pressure
Q	energy-dependent momentum-transfer cross section
$\bar{Q}$	average momentum-transfer cross section
q	independent variable
T	gas temperature
t	dummy variable of integration
v_D	ion drift velocity
x	ratio of ion-atom relative energy to kT
α	atomic polarizability
β	parameter in quadrature formula
Γ	gamma function (see appendix B)
Δ	computational error in quantity that follows
ϵ	ion-atom relative energy
$\mathcal{K}$	numerical constant, 2.492...
λ	ion mean free path
μ	ion mobility
$\bar{\sigma}$	average collision cross section
σ_x	charge exchange cross section
ψ	psi function (see appendix B)
ψ^B	Bateman's psi function (see appendix B)

Subscripts:

i	summation index in quadrature formula
m	maximum energy for which theoretical charge exchange cross section expression is valid
N	upper limit of summation in obtaining limiting values of I_2
n	summation index in obtaining limiting values of I_2

APPENDIX B

GAMMA AND MULTIGAMMA FUNCTIONS

The gamma and multigamma functions are particularly useful in determining definite integrals whose integrands contain exponential and logarithmic functions. The definition of these functions differs slightly among various texts; the differences and their relation to notation used in this report are the subject of this appendix. Most authors agree that the gamma function is defined by

$$\Gamma(q) = \int_0^\infty e^{-t} t^{q-1} \, dt \tag{B1}$$

and consequently that its relation to the factorial function is

$$q! = \Gamma(q + 1) = q\Gamma(q) \tag{B2}$$

When the various functions used to denote derivatives of the gamma and factorial functions are considered, however, little consistency is observed. Jahnke and Emde (ref. 23) define a psi function $\psi(q)$ that is identical with Jefferys' (ref. 24) digamma function $F(q)$:

$$\psi(q) = F(q) = \frac{d}{dq} (\ln q!) = \frac{1}{q!} \frac{d}{dq} (q!) \tag{B3}$$

When $q = 0$,

$$\psi(0) \equiv -\mathcal{E} = -0.577215\ldots \tag{B4}$$

where $\mathcal{E}$ is Euler's (or Mascheroni's) constant. The series for $\psi(q)$ when the argument is a positive integer n is (ref. 23)

$$\psi(n) = -\mathcal{E} + 1 + \frac{1}{2} + \frac{1}{3} + \ldots + \frac{1}{n} \tag{B5}$$

The trigamma function is defined (ref. 18) by

$$\frac{dF(q)}{dq} = \left[\frac{d\psi(q)}{dq}\right]_{q=n} = \frac{\pi^2}{6} - \left(\frac{1}{1^2} + \frac{1}{2^2} + \ldots + \frac{1}{n^2}\right) \tag{B6}$$

Bateman (ref. 17), however, defines a psi function $\psi^B(q)$ by

$$\psi^B(q) = \frac{d}{dq}\left[\ln \Gamma(q)\right] = \frac{1}{\Gamma(q)} \frac{d}{dq} \Gamma(q) \tag{B7}$$

and then generalizes it to obtain the multigamma function

$$\frac{d^n \psi^B(q)}{dq^n} = \frac{d^{n+1}}{dq^{n+1}}\left[\ln \Gamma(q)\right]$$

Hence

$$\psi(q) = \frac{1}{q\Gamma(q)} \frac{d}{dq}\left[q\Gamma(q)\right] = \frac{1}{\Gamma(q)} \frac{d}{dq}\left[\Gamma(q)\right] + \frac{1}{q} \tag{B8}$$

$$\psi(q) = \psi^B(q) + \frac{1}{q} \tag{B9}$$

For the specific case $q = 3$

$$\psi^B(3) = \psi(3) - \frac{1}{3} = -\mathscr{E} + 1 + \frac{1}{2} + \frac{1}{3} - \frac{1}{3} = \frac{3}{2} - \mathscr{E} \tag{B10}$$

The derivatives of the gamma function can be obtained by rearrangement of equations (B7) and (B9) and successive differentiations. Then

$$\frac{d\Gamma(q)}{dq} = \Gamma(q)\psi^B(q) = \Gamma(q)\left[\psi(q) - \frac{1}{q}\right] \tag{B11}$$

and

$$\frac{d^2\Gamma(q)}{dq^2} = \Gamma(q)\left\{\frac{d\psi^B(q)}{dq} - \left[\psi^B(q)\right]^2\right\} = \Gamma(q)\left\{\frac{d\psi(q)}{dq} - \left[\psi(q)\right]^2 + \frac{2\psi(q)}{q}\right\} \tag{B12}$$

Setting $q = 3$ in equation (B12) determines $\mathscr{K}$ in equation (14)

$$\mathscr{K} = \left[\frac{d^2\Gamma(q)}{dq^2}\right]_{q=3} = \Gamma(3)\left\{\left[\frac{d\psi(q)}{dq}\right]_{q=3} - \left[\psi(3)\right]^2 + \frac{2\psi(3)}{3}\right\} = 2.492927\ldots \tag{B13}$$

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